

=> fil casreact
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FILE CONTENT:1840 - 28 Sep 2008 VOL 149 ISS 14

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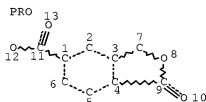
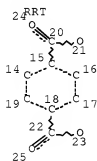
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*****
*
*   CASREACT now has more than 15.3 million reactions
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=> d que 15

L3 STR



NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 28

STEREO ATTRIBUTES: NONE
 L5 8 SEA FILE=CASREACT SSS FUL L3 (13 REACTIONS)

=> fil cap
 FILE 'CAPLUS' ENTERED AT 15:14:44 ON 29 SEP 2008
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FILE COVERS 1907 - 29 Sep 2008 VOL 149 ISS 14
 FILE LAST UPDATED: 28 Sep 2008 (20080928/ED)

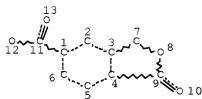
Caplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/legal/infopolicy.html>

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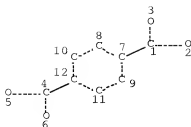
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STEREO ATTRIBUTES: NONE
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 L19 8 SEA FILE=CAPLUS ABB=ON PLU=ON L18 AND L17
 L20 1 SEA FILE=REGISTRY ABB=ON PLU=ON L2 OR 8014-95-7/CRN
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 L23 3 SEA FILE=CAPLUS ABB=ON PLU=ON L21 AND L8 AND (L11 OR L16)
 L24 8 SEA FILE=CAPLUS ABB=ON PLU=ON L19 OR L22 OR L23

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 PROCESSING COMPLETED FOR L5
 PROCESSING COMPLETED FOR L24

L25 11 DUP REM L5 L24 (5 DUPLICATES REMOVED)
 ANSWERS '1-8' FROM FILE CASREACT
 ANSWERS '9-11' FROM FILE CAPLUS

=> d l25 ibib abs crd 1-8;d l25 ibib abs hitstr 9011

L25 ANSWER 1 OF 11 CASREACT COPYRIGHT 2008 ACS on STN DUPLICATE 1
 ACCESSION NUMBER: 147:52790 CASREACT Full-text

TITLE: Multi-step process for the preparation of 5-cyanophthalide from terephthalic acid and paraformaldehyde

INVENTOR(S): Mahavir, Arora Sunil

PATENT ASSIGNEE(S): Ipca Laboratories Limited, India

SOURCE: Indian Pat. Appl., 9pp.
CODEN: INXXBQ

DOCUMENT TYPE: Patent

LANGUAGE: English

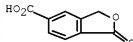
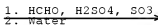
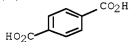
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

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IN 2003MU01074	A	20050909	IN 2003-MU1074	20031016
PRIORITY APPLN. INFO.:			IN 2003-MU1074	20031016

AB A multi-step process for the preparation of 5-cyanophthalide from terephthalic acid and paraformaldehyde is presented.

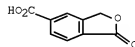
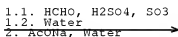
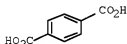
RX(1) OF 6



(step 1)

NOTE: paraformaldehyde used
CON: STAGE(1) room temperature -> 100 deg C; 3 hours; 2 hours,
110 - 120 deg C; 120 deg C -> room temperature
STAGE(2) cooled

RX(4) OF 6 - 2 STEPS



Na

NOTE: 1) paraformaldehyde used
CON: STEP(1,1) room temperature -> 100 deg C; 3 hours; 2 hours,
110 - 120 deg C; 120 deg C -> room temperature
STEP(1,2) cooled
STEP(2) room temperature -> 80 deg C

L25 ANSWER 2 OF 11 CASREACT COPYRIGHT 2008 ACS on STN DUPLICATE 2

ACCESSION NUMBER: 145:335870 CASREACT [Full-text](#)

TITLE: Synthesis of citalopram hydrobromide

AUTHOR(S): Wu, Qiuye; Liao, Hongli; Zhao, Huiqing; Ye, Guangming; Jin, Yongsheng

CORPORATE SOURCE: School of Pharmacy, Second Military Medical University, Shanghai, 200433, Peop. Rep. China

SOURCE: Zhongguo Yiyao Gongye Zazhi (2005), 36(1), 6-8
CODEN: ZYGZEA; ISSN: 1001-8255

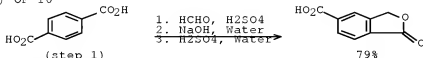
PUBLISHER: Zhongguo Yiyao Gongye Zazhi Bianjibu

DOCUMENT TYPE: Journal

LANGUAGE: Chinese

AB Citalopram hydrobromide [i.e., 1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-5-isobenzofurancarbonitrile monohydrobromide] was synthesized from terephthalic acid and paraformaldehyde by condensation to give 5-carboxyphthalanone, which subjected to condensation, amidation and dehydration to afford 5-cyanophthalanone followed by twice Grignard reaction, cyclization and then salification with an overall yield of 31%.

RX(2) OF 10



NOTE: paraformaldehyde used

CON: STAGE(1) room temperature -> 142 deg C; 5 hours, 142 deg C

STAGE(2) pH 7

STAGE(3) pH 2

L25 ANSWER 3 OF 11 CASREACT COPYRIGHT 2008 ACS on STN DUPLICATE 3

ACCESSION NUMBER: 141:314145 CASREACT [Full-text](#)

TITLE: Preparation of 5-alkoxycarbonylphthalides as intermediates for the preparation of citalopram and escitalopram

INVENTOR(S): Pittelkow, Thomas; Castellin, Andrea; Sbrogio, Federico; Dahlberg, Nielsen Poul; Zanon, Jacopo; Soegaard, Steen; Humble, Rikke Eva

PATENT ASSIGNEE(S): H. Lundbeck A/S, Den.

SOURCE: PCT Int. Appl., 31 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

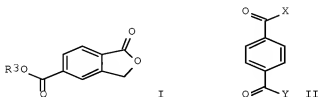
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WO 2004083197	A3	20041028		
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RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2519629	A1	20040930	CA 2004-2519629	20040317
EP 1611118	A2	20060104	EP 2004-721125	20040317
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK				
CN 1761659	A	20060419	CN 2004-80007510	20040317
IN 2005CN02322	A	20070302	IN 2005-CN2322	20050920

US 20080058536
PRIORITY APPLN. INFO.:

A1 20080306

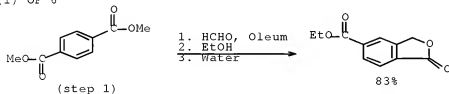
US 2007-550419 20070530
DK 2003-440 20030321
US 2003-456415P 20030321
WO 2004-DK177 20040317

OTHER SOURCE(S): MARPAT 141:314145
GI

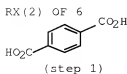


AB Methods for manufacture of 5-alkoxycarbonylphthalides (I; R3 = C1-6 alkyl, Ph) are disclosed, which comprise (a) reaction of terephthalic acid derivs. (II; X, Y = OR1, OR2 Cl, Br, iodo, NHR; R-R2 = independently H or C1-6 alkyl) with formaldehyde or its equivalent (trioxane or paraformaldehyde) or oleum and (b) addition of an alc. R3-OH to the reaction of step (a). The 5-alkoxycarbonylphthalides are useful in syntheses of the well-known antidepressants citalopram and escitalopram. Thus, oleum (20-25% SO3, 160 L) was charged into a glass reactor (400 L) and under stirring di-Me terephthalate (90.7 kg) was added to the reactor, followed by adding paraformaldehyde (18.6 kg). The reaction mixture was agitated at 125° for 5 h, cooled to 70°, and added to a reactor containing ethanol (620 L) at ambient temperature about 20°. The mixture was heated at 85-93° for 1.5 h and then cooled to approximated 80° before ice (240 kg) was added. After stirring overnight the mixture was cooled to 15° and the precipitate was filtered off and washed with water (150 L). The crude product was added to a stirred mixture of water (250 L) and to this slurry was added NaOH (27.7%, approximated 250 L) to a pH about 4. The precipitate was filtered off and washed with water (500 L) and dried to give 83% 5-ethoxycarbonylphthalide.

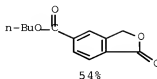
RX(1) OF 6



NOTE: pilot plant, scalable, paraformaldehyde was used
CON: STAGE(1) room temperature; 5 hours, 125 deg C;
15 deg C -> 70 deg C
STAGE(2) 1.5 hours, 85-93 deg C; 93 deg C -> 80 deg C

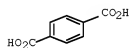


1. Oleum
2. Formaldehyde trimer
3. BuOH, Heptane

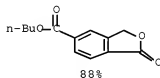


NOTE: optimization study, thermal
CON: STAGE(1) room temperature -> 60 deg C; 30 minutes; 60 minutes,
100 deg C; 100 deg C -> 30 deg C
STAGE(2) 1.5 hours 130 - 135 deg C; 4 hours, 155 deg C;
155 deg C -> 40 deg C

RX(6) OF 6 - 2 STEPS



1.1. HCHO, Oleum
1.2. Water
2. BuOH, H2SO4, PhMe,
Water



NOTE: 1) paraformaldehyde was used, thermal
CON: STEP(1) room temperature -> 150 deg C; 2 hour, 150 deg C;
4 hours, 150 deg C; 150 deg C -> 90 deg C
STEP(1,2) <100 deg C
STEP(2) room temperature -> 85 deg C

L25 ANSWER 4 OF 11 CASREACT COPYRIGHT 2008 ACS on STN DUPLICATE 4

ACCESSION NUMBER: 134:326395 CASREACT [Full-text](#)

TITLE: Regioselective preparation of 5-carboxyphthalide by the cyclocondensation of terephthalic acid with paraformaldehyde in oleum

INVENTOR(S): Petersen, Hans; Dahlberg, Nielsen Poul

PATENT ASSIGNEE(S): H. Lundbeck A/S, Den.

SOURCE: PCT Int. Appl., 9 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001032642	A1	20010510	WO 2000-DK585	20001019
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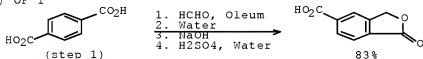
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CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

CA 2389379 A1 20010510 CA 2000-2389379 20001019
CA 2389379 C 20070410
US 6403813 B1 20020611 US 2000-692653 20001019
BR 2000015471 A 20020709 BR 2000-15471 20001019
EP 1235819 A1 20020904 EP 2000-969234 20001019
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JP 2003513084 T 20030408 JP 2001-534793 20001019
IT 1319251 B1 20030926 IT 2000-MI2342 20001027
MX 2002PA04313 A 20021107 MX 2002-PA4313 20020430
US 20020165403 A1 20021107 US 2002-140361 20020506
US 6888009 B2 20050503
IN 2002CN00774 A 20050520 IN 2002-CN774 20020524
HK 1052702 A1 20050923 HK 2003-104993 20030710
DK 1999-1569 19991101
US 2000-692653 20001019
WO 2000-DK585 20001019

PRIORITY APPLN. INFO.:

AB 5-Carboxyphthalide, a pharmaceutical intermediate, is prepared, on an industrial scale, in very high yield and purity by a the regioselective cyclocondensation of terephthalic acid with paraformaldehyde in the presence of oleum.

RX(1) OF 1



NOTE: paraformaldehyde used

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 5 OF 11 CASREACT COPYRIGHT 2008 ACS on STN DUPLICATE 5
ACCESSION NUMBER: 135:107244 CASREACT [Full-text](#)
TITLE: High-yield process for the preparation of 5-carboxyphthalide by the reaction of terephthalic acid with formaldehyde in the presence of oleum
INVENTOR(S): Dall'Asta, Leone; Casazza, Umberto; Cotticelli, Giovanni
PATENT ASSIGNEE(S): Norpharma S.p.A., Italy
SOURCE: Eur. Pat. Appl., 6 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

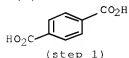
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EP 1118614 B1 20020619
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
 IE, SI, LT, LV, FI, RO
 IT 2000MI0050 A1 20010718 IT 2000-MI50 20000118
 IT 1317729 B1 20030715
 AT 219489 T 20020715 AT 2000-203602 20001017
 PT 1118614 T 20021129 PT 2000-203602 20001017
 ES 2178626 T3 20030101 ES 2000-203602 20001017
 JP 2001206881 A 20010731 JP 2000-372224 20001207
 CA 2397497 A1 20010726 CA 2001-2397497 20010117
 WO 2001053284 A1 20010726 WO 2001-EF617 20010117
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 AU 2001026798 A 20010731 AU 2001-26798 20010117
 AU 779581 B2 20050127
 EP 1187822 A1 20020320 EP 2001-901181 20010117
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 BR 2001007853 A 20021029 BR 2001-7853 20010117
 HU 2002004187 A2 20030328 HU 2002-4187 20010117
 HU 2002004187 A3 20050530
 RO 121737 B1 20080328 RO 2002-989 20010117
 HK 1042290 A1 20030718 HK 2002-100631 20020125
 ZA 2002005475 A 20031010 ZA 2002-5475 20020709
 IN 2002KN00905 A 20050701 IN 2002-KN905 20020709
 BG 106925 A 20040130 BG 2002-106925 20020716
 MX 2002PA07031 A 20040906 MX 2002-PA7031 20020718
 US 20030009038 A1 20030109 US 2002-227038 20020823
 US 6703516 B2 20040309
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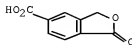
PRIORITY APPLN. INFO.:

AB A process for the preparation of 5-carboxyphthalide comprises adding terephthalic acid to fuming sulfuric acid (i.e., oleum) containing $\geq 20\%$ of SO_3 , then adding formaldehyde to the mixture, heating it at $120-145^\circ$, and isolating 5-carboxyphthalide.

RX(1) OF 1

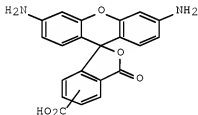


1. Formaldehyde trimer,
Oleum
2. AcOH, Water
3. NaHCO_3 , Water
4. HCl , Water



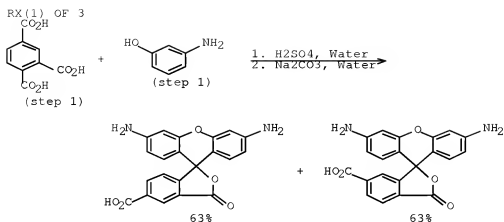
ACCESSION NUMBER: 142:156327 CASREACT Full-text
 TITLE: Methods for the preparation of rhodamine for use in peptide synthesis
 INVENTOR(S): Damoiseaux, Robert D.; Harris, Jennifer L.
 PATENT ASSIGNEE(S): IRM LLC, Bermuda
 SOURCE: PCT Int. Appl., 29 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2005007678	A2	20050127	WO 2004-US22775	20040714
WO 2005007678	A3	20050407		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 20050113584	A1	20050526	US 2004-891826	20040714
PRIORITY APPLN. INFO.:			US 2003-487331P	20030714
OTHER SOURCE(S):			MARPAT 142:156327	
GI				



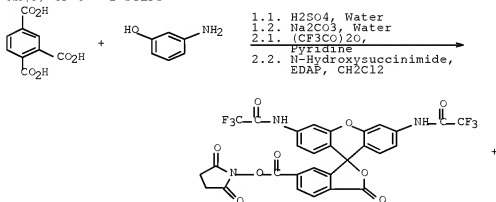
I

AB The invention relates to a method for preparing rhodamine (I) on a solid support and, in particular, methods for the economical preparation of rhodamine NHS ester. The attachment of rhodamine NHS ester to a solid support and use of the rhodamine free amines as attachment points for peptides is especially attractive in peptide chemical and in screening assays for protease activity. Thus, stirring a mixture of 1,2,4-benzenetricarboxylic acid and 3-aminophenol in H2SO4 at 180°C for 6 h afforded 63% rhodamine of about 90% purity.

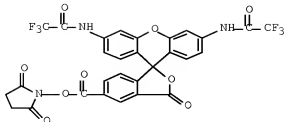


NOTE: thermal
CON: STAGE(1) room temperature; room temperature -> 180 deg C;
6 hours, 180 deg C; cooled
STAGE(2) neutralized

RX(3) OF 3 - 2 STEPS



RX (3) OF 3 - 2 STEPS

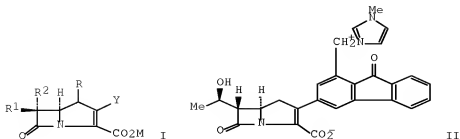


NOTE: 1) thermal, 2) combined yield of 14%
 CON: STEP(1.1) room temperature; room temperature -> 180 deg C;
 6 hours, 180 deg C; cooled
 STEP(1.2) neutralized
 STEP(2.1) room temperature; overnight, room temperature
 STEP(2.2) room temperature; 35 minutes, room temperature

L25 ANSWER 7 OF 11 CASREACT COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 116:59077 CASREACT Full-text
 TITLE: Preparation of 2-(9-fluorenonyl)carbapenem
 antibacterial agents
 INVENTOR(S): Greenlee, Mark L.; DiNinno, Frank P.; Cama, Lovji D.;
 Heck, James V.
 PATENT ASSIGNEE(S): Merck and Co., Inc., USA
 SOURCE: U.S., 85 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 3
 PATENT INFORMATION:

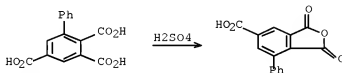
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5034384	A	19910723	US 1990-561547	19900801
EP 472306	A1	19920226	EP 1991-306955	19910730
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
FI 9103655	A	19920202	FI 1991-3655	19910731
NO 9102980	A	19920203	NO 1991-2980	19910731
AU 9181517	A	19920206	AU 1991-81517	19910731
AU 642518	B2	19931021		
ZA 9106019	A	19920429	ZA 1991-6019	19910731
JP 05105679	A	19930427	JP 1991-280913	19910731
JP 2509771	B2	19960626		
CA 2048269	A1	19920202	CA 1991-2048269	19910801
US 5356889	A	19941018	US 1992-966969	19921026
PRIORITY APPLN. INFO.:			US 1990-561547	19900801
			US 1990-594808	19901009

OTHER SOURCE(S): MARPAT 116:59077
 GI

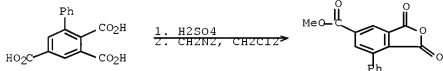


AB The title compds. [I; M = H, ester residue, alkali metal cation, neg. charge, etc.; R = H, Me; R1, R2 = H, Me, Et, CH2OH, MeCH(OH), etc.; Y = 9-fluorenon-2- or -3-yl optionally substituted by, e.g., 1-methylimidazolium-3-ylmethyl, 4-amino-1,2,4-triazolium-1-ylmethyl, 2-aminopyridinium-1-ylmethyl, etc.] were prepared as antibiotics (no data). Thus, 4-nitrobenzyl (5R,6S)-2-oxo-6-[(1R)-hydroxyethyl]carbapenem-3- carboxylate was condensed with 3-trimethylstannyl-1-hydroxymethyl-9- fluorenone (preparation given) and the product condensed with 1-methylimidazole to give, after deprotection, title compound II.

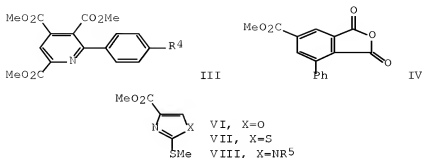
RX(4) OF 232



RX(48) OF 232 - 2 STEPS

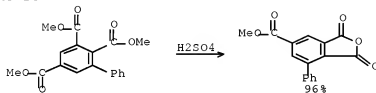


L25 ANSWER 8 OF 11 CASREACT COPYRIGHT 2008 ACS on SIN
 ACCESSION NUMBER: 95:7151 CASREACT [Full-text](#)
 TITLE: New 4-amino-2-azabutadienes and 1-aminobutadienes: synthesis from pyridines, benzenes, and azoles
 AUTHOR(S): Gompper, Rudolf; Heinemann, Ulrich
 CORPORATE SOURCE: Inst. Org. Chem., Univ. Muenchen, Munich, D-8000/2, Fed. Rep. Ger.
 SOURCE: Angewandte Chemie (1981), 93(3), 297-8
 CODEN: ANCEAD; ISSN: 0044-8249
 DOCUMENT TYPE: Journal
 LANGUAGE: German
 GI



AB R1CH2N:CR2R3 [R1 = CO2Me, cyano; R2 = H, Me; R3 = 4-R4C6H4 (R4 = H, Cl, Me, Me2N), SMe, NMe2] heated with HC(OEt)2NMe2 [or [Me2NCHCl]+ Cl- for MeO2CCH2N:CHNMe2] gave 35-87% Me2NCH:CR1N:CR2R3 (I). A mixture of MeO2CCH2CH:CHPh and MeO2CCH:CHCH2Ph similarly gave 71% Me2NCH:C(CO2Me)CH:CHPh (II). I (R1 = CO2Me, R2 = H, R3 = H, Cl, Me) cyclized with MeO2CC.tpbond.CO2Me to give 15-41% pyridines III, and II gave 35% 2,3,5-(MeO2C)3C6H2Ph, which gave 96% anhydride IV with concentrated H2SO4. Boiling II (R1 = CO2Me, R2 = R3 = SMe) (V) in THF-dilute HCl gave 86% oxazole VI, whereas passing HCl through V in THF at 20°, then H2S while heating the mixture gave 85% thiazole VII. Heating V with R5NH2.HCl (R5 = Ph, CH2Ph) in dioxane-DMF gave 22-38% imidazoles VIII.

RX(13) OF 24



11 ANSWERS ARE AVAILABLE. SPECIFIED ANSWER NUMBER EXCEEDS ANSWER SET SIZE
The answer numbers requested are not in the answer set.
ENTER ANSWER NUMBER OR RANGE (1):9-11

L25 ANSWER 9 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:534492 CAPLUS [Full-text](#)
DOCUMENT NUMBER: 145:29562
TITLE: Water-thinned polyester-based resin compositions for coating of cans, and coated metal sheets
INVENTOR(S): Tajika, Hiroshi
PATENT ASSIGNEE(S): Toyobo Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 19 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1

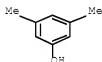
PATENT INFORMATION:

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	JP 2006143891	A	20060608	JP 2004-335972	20041119
PRIORITY APPLN. INFO.:				JP 2004-335972	20041119
AB	The resin compns. contain polyesters (A) (acid value 150-800 equiv/106 g, Mn 5,000-100,000) consisting of polycarboxylic acid components containing 70-100 mol% aromatic dicarboxylic acids and 0-30 mol% other polycarboxylic acids and polyol components containing 40-100 mol% (in total) 2-ethyl-2-butyl-1,3-propanediol and 2-methyl-1,3-propanediol, 1,4-butanediol, and/or 1,4-cyclohexanedimethanol and 0-60 mol% other polyols, resol-type phenolic resins (B), basic compds. (C), and H ₂ O. Thus, a water-thinned coating composition containing 85 parts of 30:69:4:20:55:25 (by mol) terephthalic acid-isophthalic acid-trimellitic anhydride-2-ethyl-2-butyl-1,3-propanediol-1,4-butanediol-1,4-cyclohexanedimethanol copolymer (Mn 15,000, acid value 230 equiv/106 g), 15 parts resol-type m-cresol-formaldehyde copolymer, and 2.1 parts N,N-dimethylethanolamine was applied on an Al sheet (5052) and baked to give a coated test piece showing good curability, workability, overbake resistance, retort resistance, acid resistance, and dent resistance.				
IT	25086-35-5P, Formaldehyde-3,5-xyleneol copolymer 25086-36-6P, m-Cresol-formaldehyde copolymer RL: IMF (Industrial manufacture); RCT (Reactant); TEM (Technical or engineered material use); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (resol, crosslinking agent; water-thinned coatings containing polyesters, resols, and basic compds. for coated metal cans with good workability, overbake resistance, and retort resistance)				
RN	25086-35-5 CAPLUS				
CN	Formaldehyde, polymer with 3,5-dimethylphenol (CA INDEX NAME)				

CM 1

CRN 108-68-9

CMF C8 H10 O



CM 2

CRN 50-00-0

CMF C H2 O

H₂C=O

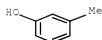
RN 25086-36-6 CAPLUS

CN Formaldehyde, polymer with 3-methylphenol (CA INDEX NAME)

CM 1

CRN 108-39-4

CMF C7 H8 O



CM 2

CRN 50-00-0

CMF C H2 O



IT 889651-66-5P 889651-68-7P 889651-70-1P

889651-72-3P

RL: IMF (Industrial manufacture); RCT (Reactant); TEM
(Technical or engineered material use); PREP (Preparation);

RACT (Reactant or reagent); USES (Uses)

(water-thinned coatings containing polyesters, resols, and basic compds.
for coated metal cans with good workability, overbake resistance, and
retort resistance)

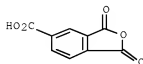
RN 889651-66-5 CAPLUS

CN 1,3-Benzenedicarboxylic acid, polymer with 1,4-benzenedicarboxylic acid,
1,4-butanediol, 2-butyl-2-ethyl-1,3-propanediol, 1,4-cyclohexanedimethanol
and 1,3-dihydro-1,3-dioxo-5-isobenzofurancarboxylic acid (9CI) (CA INDEX
NAME)

CM 1

CRN 552-30-7

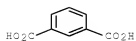
CMF C9 H4 O5



CM 2

CRN 121-91-5

CMF C8 H6 O4



CM 3

CRN 115-84-4

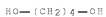
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CM 4

CRN 110-63-4

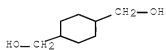
CMF C4 H10 O2



CM 5

CRN 105-08-8

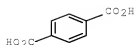
CMF C8 H16 O2



CM 6

CRN 100-21-0

CMF C8 H6 O4



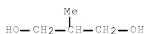
RN 889651-68-7 CAPLUS

CN 1,3-Benzenedicarboxylic acid, polymer with 1,4-benzenedicarboxylic acid, 1,4-butanediol, 2-butyl-2-ethyl-1,3-propanediol, 1,3-dihydro-1,3-dioxo-5-isobenzofurancarboxylic acid, 1,2-ethanediyl bis(1,3-dihydro-1,3-dioxo-5-isobenzofurancarboxylate) and 2-methyl-1,3-propanediol (9CI) (CA INDEX NAME)

CM 1

CRN 2163-42-0

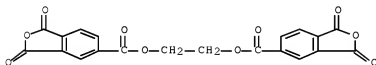
CMF C4 H10 O2



CM 2

CRN 1732-96-3

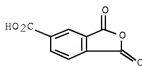
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CM 3

CRN 552-30-7

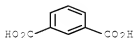
CMF C9 H4 O5



CM 4

CRN 121-91-5

CMF C8 H6 O4



CM 5

CRN 115-84-4

CMF C9 H20 O2



CM 6

CRN 110-63-4

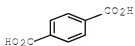
CMF C4 H10 O2



CM 7

CRN 100-21-0

CMF C8 H6 O4



RN 889651-70-1 CAPLUS

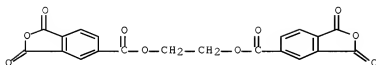
CN 1,3-Benzenedicarboxylic acid, polymer with 1,4-benzenedicarboxylic acid, 2-butyl-2-ethyl-1,3-propanediol, 1,4-cyclohexanedimethanol, decanedioic acid, 1,3-dihydro-1,3-dioxo-5-isobenzofurancarboxylic acid, 1,2-ethanediol and 1,2-ethanediyl bis(1,3-dihydro-1,3-dioxo-5-isobenzofurancarboxylate)

(9CI) (CA INDEX NAME)

CM 1

CRN 1732-96-3

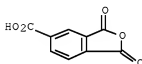
CMF C20 H10 O10



CM 2

CRN 552-30-7

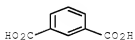
CMF C9 H4 O5



CM 3

CRN 121-91-5

CMF C8 H6 O4



CM 4

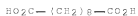
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CMF C9 H20 O2



CM 5

CRN 111-20-6
 CMF C10 H18 O4



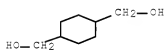
CM 6

CRN 107-21-1
 CMF C2 H6 O2



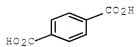
CM 7

CRN 105-08-8
 CMF C8 H16 O2



CM 8

CRN 100-21-0
 CMF C8 H6 O4



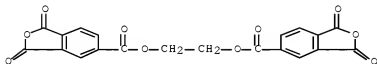
RN 889651-72-3 CAPLUS
 CN 1,3-Benzenedicarboxylic acid, polymer with 1,4-benzenedicarboxylic acid,
 1,4-butanediol, 2-butyl-2-ethyl-1,3-propanediol, 1,4-
 cyclohexanedimethanol, 1,3-dihydro-1,3-dioxo-5-isobenzofurancarboxylic

acid, 1,2-ethanediyl bis(1,3-dihydro-1,3-dioxo-5-isobenzofurancarboxylate)
and 4-hydroxy- γ -(4-hydroxyphenyl)- γ -methylbenzenebutanoic acid
(9CI) (CA INDEX NAME)

CM 1

CRN 1732-96-3

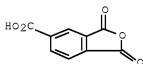
CMF C20 H10 O10



CM 2

CRN 552-30-7

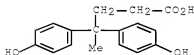
CMF C9 H4 O5



CM 3

CRN 126-00-1

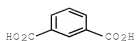
CMF C17 H18 O4



CM 4

CRN 121-91-5

CMF C8 H6 O4



CM 5

CRN 115-84-4

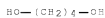
CMF C9 H20 O2



CM 6

CRN 110-63-4

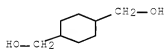
CMF C4 H10 O2



CM 7

CRN 105-08-8

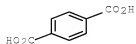
CMF C8 H16 O2



CM 8

CRN 100-21-0

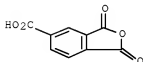
CMF C8 H6 O4



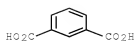
IT 889651-75-6P 889651-78-9P 889651-81-4P
 889651-83-6P
 RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
 (water-thinned coatings containing polyesters, resols, and basic compds. for coated metal cans with good workability, overbake resistance, and retort resistance)
 RN 889651-75-6 CAPLUS
 CN 1,3-Benzenedicarboxylic acid, polymer with 1,4-benzenedicarboxylic acid, 1,4-butanediol, 2-butyl-2-ethyl-1,3-propanediol, 1,4-cyclohexanedimethanol, 1,3-dihydro-1,3-dioxo-5-isobenzofurancarboxylic acid, formaldehyde and 3-methylphenol, compd. with 2-(dimethylamino)ethanol (9CI) (CA INDEX NAME)
 CM 1
 CRN 108-01-0
 CMF C4 H11 N O

Me2N-CH2-CH2-OH

CM 2
 CRN 889651-74-5
 CMF (C9 H20 O2 . C9 H4 O5 . C8 H16 O2 . C8 H6 O4 . C8 H6 O4 . C7 H8 O . C4 H10 O2 . C H2 O)x
 CCI PMS
 CM 3
 CRN 552-30-7
 CMF C9 H4 O5



CM 4
 CRN 121-91-5
 CMF C8 H6 O4



CM 5

CRN 115-84-4

CMF C9 H20 O2



CM 6

CRN 110-63-4

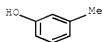
CMF C4 H10 O2



CM 7

CRN 108-39-4

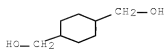
CMF C7 H8 O



CM 8

CRN 105-08-8

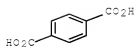
CMF C8 H16 O2



CM 9

CRN 100-21-0

CMF C8 H6 O4



CM 10

CRN 50-00-0

CMF C H2 O



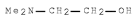
RN 889651-78-9 CAPLUS

CN 1,3-Benzenedicarboxylic acid, polymer with 1,4-benzenedicarboxylic acid, 1,4-butanediol, 2-butyl-2-ethyl-1,3-propanediol, 1,3-dihydro-1,3-dioxo-5-isobenzofurancarboxylic acid, 1,2-ethanediyl bis(1,3-dihydro-1,3-dioxo-5-isobenzofurancarboxylate), formaldehyde, 3-methylphenol and 2-methyl-1,3-propanediol, compd. with 2-(dimethylamino)ethanol (9CI) (CA INDEX NAME)

CM 1

CRN 108-01-0

CMF C4 H11 N O



CM 2

CRN 889651-77-8

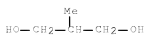
CMF (C20 H10 O10 . C9 H20 O2 . C9 H4 O5 . C8 H6 O4 . C8 H6 O4 . C7 H8 O . C4 H10 O2 . C4 H10 O2 . C H2 O)x

CCI PMS

CM 3

CRN 2163-42-0

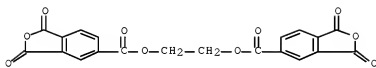
CMF C4 H10 O2



CM 4

CRN 1732-96-3

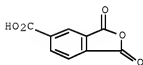
CMF C20 H10 O10



CM 5

CRN 552-30-7

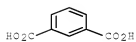
CMF C9 H4 O5



CM 6

CRN 121-91-5

CMF C8 H6 O4



CM 7

CRN 115-84-4

CMF C9 H20 O2



CM 8

CRN 110-63-4

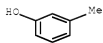
CMF C4 H10 O2



CM 9

CRN 108-39-4

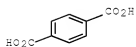
CMF C7 H8 O



CM 10

CRN 100-21-0

CMF C8 H6 O4



CM 11

CRN 50-00-0

CMF C H2 O

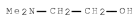


RN 889651-81-4 CAPLUS
 CN 1,3-Benzenedicarboxylic acid, polymer with 1,4-benzenedicarboxylic acid, 2-butyl-2-ethyl-1,3-propanediol, 1,4-cyclohexanedimethanol, decanedioic acid, 1,3-dihydro-1,3-dioxo-5-isobenzofurancarboxylic acid, 3,5-dimethylphenol, 1,2-ethanediol, 1,2-ethanediyl bis(1,3-dihydro-1,3-dioxo-5-isobenzofurancarboxylate) and formaldehyde, compd. with 2-(dimethylamino)ethanol (9CI) (CA INDEX NAME)

CM 1

CRN 108-01-0

CMF C4 H11 N O



CM 2

CRN 889651-80-3

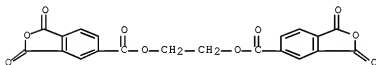
CMF (C20 H10 O10 . C10 H18 O4 . C9 H20 O2 . C9 H4 O5 . C8 H16 O2 . C8 H10 O . C8 H6 O4 . C8 H6 O4 . C2 H6 O2 . C H2 O)x

CCI PMS

CM 3

CRN 1732-96-3

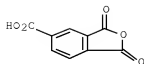
CMF C20 H10 O10



CM 4

CRN 552-30-7

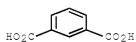
CMF C9 H4 O5



CM 5

CRN 121-91-5

CMF C8 H6 O4



CM 6

CRN 115-84-4

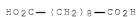
CMF C9 H20 O2



CM 7

CRN 111-20-6

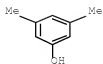
CMF C10 H18 O4



CM 8

CRN 108-68-9

CMF C8 H10 O



CM 9

CRN 107-21-1

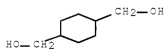
CMF C2 H6 O2



CM 10

CRN 105-08-8

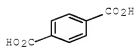
CMF C8 H16 O2



CM 11

CRN 100-21-0

CMF C8 H6 O4



CM 12

CRN 50-00-0

CMF C H2 O



RN 889651-83-6 CAPLUS
 CN 1,3-Benzenedicarboxylic acid, polymer with 1,4-benzenedicarboxylic acid, 1,4-butanediol, 2-butyl-2-ethyl-1,3-propanediol, 1,4-cyclohexanedimethanol, 1,3-dihydro-1,3-dioxo-5-isobenzofurancarboxylic acid, 3,5-dimethylphenol, 1,2-ethanediyl bis(1,3-dihydro-1,3-dioxo-5-isobenzofurancarboxylate), formaldehyde and 4-hydroxy-γ-(4-hydroxyphenyl)-γ-methylbenzenebutanoic acid, compd. with 2-(dimethylamino)ethanol (9CI) (CA INDEX NAME)

CM 1

CRN 108-01-0

CMF C4 H11 N O



CM 2

CRN 889651-82-5

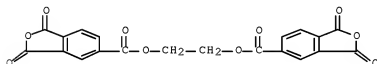
CMF (C20 H10 O10 . C17 H18 O4 . C9 H20 O2 . C9 H4 O5 . C8 H16 O2 . C8 H10 O . C8 H6 O4 . C8 H6 O4 . C4 H10 O2 . C H2 O)x

CCI PMS

CM 3

CRN 1732-96-3

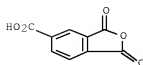
CMF C20 H10 O10



CM 4

CRN 552-30-7

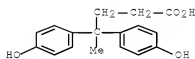
CMF C9 H4 O5



CM 5

CRN 126-00-1

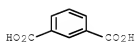
CMF C17 H18 O4



CM 6

CRN 121-91-5

CMF C8 H6 O4



CM 7

CRN 115-84-4

CMF C9 H20 O2



CM 8

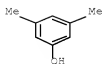
CRN 110-63-4

CMF C4 H10 O2



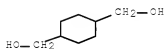
CM 9

CRN 108-68-9
CMF C8 H10 O



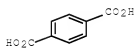
CM 10

CRN 105-08-8
CMF C8 H16 O2



CM 11

CRN 100-21-0
CMF C8 H6 O4



CM 12

CRN 50-00-0
CMF C H2 O



L25 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:338514 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 134:326396

TITLE: Method for the preparation of 5-carboxyphthalide from terephthalic acid and trioxane or paraformaldehyde

INVENTOR(S): Petersen, Hans
 PATENT ASSIGNEE(S): H. Lundbeck A/S, Den.
 SOURCE: PCT Int. Appl., 8 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001032643	A1	20010510	WO 2000-DK606	20001101
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, FR, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				

PRIORITY APPLN. INFO.: DK 1999-1568 A 19991101

OTHER SOURCE(S): CASREACT 134:326396

AB 5-Carboxyphthalide, useful as an antidepressant intermediate, is prepared in high yield and selectivity by the cyclocondensation reaction of terephthalic acid with trioxane or paraformaldehyde in the presence of a Lewis acid (e.g., ZnCl₂) or a mineral acid (e.g., polyphosphoric acid).

IT 100-21-0, Terephthalic acid, reactions 110-88-3,
 1,3,5-Trioxane, reactions 30525-89-4, Paraformaldehyde

RL: RCT (Reactant); RACT (Reactant or reagent)

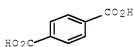
(method for the preparation of 5-carboxyphthalide from terephthalic acid

and

trioxane or paraformaldehyde)

RN 100-21-0 CAPLUS

CN 1,4-Benzenedicarboxylic acid (CA INDEX NAME)



RN 110-88-3 CAPLUS

CN 1,3,5-Trioxane (CA INDEX NAME)



RN 30525-89-4 CAPLUS

CN Paraformaldehyde (CA INDEX NAME)

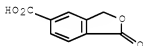
CM 1

CRN 50-00-0

CMF C H2 O

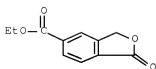
H2C=O

IT 4792-29-4P, 5-Carboxyphthalide
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (method for the preparation of 5-carboxyphthalide from terephthalic acid
 and trioxane or paraformaldehyde)
 RN 4792-29-4 CAPLUS
 CN 5-Isobenzofurancarboxylic acid, 1,3-dihydro-1-oxo- (CA INDEX NAME)

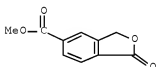


REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

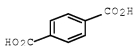
L25 ANSWER 11 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1970:403627 CAPLUS Full-text
 DOCUMENT NUMBER: 73:3627
 ORIGINAL REFERENCE NO.: 73:613a,616a
 TITLE: Reaction of terephthalic acid with formaldehyde in
 sulfur trioxide media
 AUTHOR(S): Forney, LeRoy S.
 CORPORATE SOURCE: Res. and Develop. Lab., Mobil Chem. Co., Edison, NJ,
 USA
 SOURCE: Journal of Organic Chemistry (1970), 35(5), 1695-6
 CODEN: JOCEAH; ISSN: 0022-3263
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI For diagram(s), see printed CA Issue.
 AB The title acid is treated with H2CO in SO3 at 120-30° to give 5-
 carboxyphthalide (I); 2-hydroxymethylterephthalic acid is prepared by the
 saponification of I. Excess H2CO gives p-HO2CC6H4CO2CH2CO2H.
 IT 23405-31-4P 23405-32-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 23405-31-4 CAPLUS
 CN 5-Isobenzofurancarboxylic acid, 1,3-dihydro-1-oxo-, ethyl ester (CA INDEX
 NAME)



RN 23405-32-5 CAPLUS
 CN 5-Isobenzofurancarboxylic acid, 1,3-dihydro-1-oxo-, methyl ester (CA INDEX NAME)



IT 100-21-0, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (with formaldehyde)
 RN 100-21-0 CAPLUS
 CN 1,4-Benzenedicarboxylic acid (CA INDEX NAME)



IT 50-00-0, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (with terephthalic acid)
 RN 50-00-0 CAPLUS
 CN Formaldehyde (CA INDEX NAME)



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(FILE 'HOME' ENTERED AT 14:59:19 ON 29 SEP 2008)

FILE 'CASREACT' ENTERED AT 14:59:34 ON 29 SEP 2008

FILE 'REGISTRY' ENTERED AT 14:59:40 ON 29 SEP 2008

L1 STR

FILE 'REGISTRY' ENTERED AT 15:03:54 ON 29 SEP 2008
 E FUMING SULFURIC/CN
 L2 1 SEA ABB=ON PLU=ON "FUMING SULFURIC ACID"/CN
 D SCA

FILE 'CASREACT' ENTERED AT 15:04:30 ON 29 SEP 2008
 STR L1
 L3 1 SEA SSS SAM L3 (2 REACTIONS)
 L4 8 SEA SSS FUL L3 (13 REACTIONS)
 L5

FILE 'REGISTRY' ENTERED AT 15:06:14 ON 29 SEP 2008
 STR L3
 L6 50 SEA SSS SAM L6
 L7 12145 SEA SSS FUL L6
 L8

FILE 'REGISTRY' ENTERED AT 15:07:46 ON 29 SEP 2008
 E TEREPHTHALIC ACID/CN
 L9 1 SEA ABB=ON PLU=ON "TEREPHTHALIC ACID"/CN
 D SCA
 D

FILE 'REGISTRY' ENTERED AT 15:08:42 ON 29 SEP 2008
 STR 100-21-0
 L10 27124 SEA FAM FUL L10
 L11 1 SEA ABB=ON PLU=ON FORMALDEHYDE/CN
 L12 1 SEA ABB=ON PLU=ON PARAFORMALDEHYDE/CN
 L13 1 SEA ABB=ON PLU=ON 1,3,5-TRIOXANE/CN
 L14 3 SEA ABB=ON PLU=ON (L12 OR L13 OR L14)
 L15 SEL RN
 L16 29207 SEA ABB=ON PLU=ON (110-88-3/CRN OR 30525-89-4/CRN OR
 50-00-0/CRN) OR L15

FILE 'CAPLUS' ENTERED AT 15:10:54 ON 29 SEP 2008
 L17 49 SEA ABB=ON PLU=ON L11(L)RACT+NT/RL AND L16(L)RACT+NT/RL
 L18 5714 SEA ABB=ON PLU=ON L8(L)PREP+NT/RL
 L19 8 SEA ABB=ON PLU=ON L18 AND L17

FILE 'REGISTRY' ENTERED AT 15:12:05 ON 29 SEP 2008
 SEL RN L2
 L20 1 SEA ABB=ON PLU=ON L2 OR 8014-95-7/CRN

FILE 'CAPLUS' ENTERED AT 15:12:48 ON 29 SEP 2008
 L21 567 SEA ABB=ON PLU=ON L20(L)RACT+NT/RL
 L22 3 SEA ABB=ON PLU=ON L19 AND L21
 L23 3 SEA ABB=ON PLU=ON L21 AND L8 AND (L11 OR L16)
 L24 8 SEA ABB=ON PLU=ON L19 OR L22 OR L23

FILE 'CASREACT' ENTERED AT 15:14:40 ON 29 SEP 2008
 D QUE L5

FILE 'CAPLUS' ENTERED AT 15:14:44 ON 29 SEP 2008
 D QUE L24

FILE 'CASREACT, CAPLUS' ENTERED AT 15:14:50 ON 29 SEP 2008
 L25 11 DUP REM L5 L24 (5 DUPLICATES REMOVED)
 ANSWERS '1-8' FROM FILE CASREACT
 ANSWERS '9-11' FROM FILE CAPLUS
 D L25 IBIB ABS CRD 1-8
 D L25 IBIB ABS HITSTR 9011